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Vertex-based and edge-based centroids of graphs

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ABSTRACT

The sum of distances between all pairs of vertices, better known as the Wiener index for its applications in Chemistry, has been extensively studied in the past decades. One of the most important properties related to distance between vertices, in the form of the middle part of a tree called the "centroid", has been thoroughly analyzed. Also arised in the study of Chemical Graph Theory is the edge Wiener index which studies the distances between edges. Various problems on this concept have been proposed and investigated, along with its correlation to the original Wiener index. We extend the study to the middle part of a tree in this note, showing interesting and sometimes rather unexpected observations on the so-called "edge centroid". We also shed some more light on the relations between these distance-based graph invariants by investigating the behaviors of different centroids and their differences. Such edge-centroids are also compared with the vertex-based analogues in both trees and graphs. This leads to challenging questions for future work in this direction.

1. Introduction

The sum of distances between all pairs of vertices (as a pure mathematical concept) has probably been studied much earlier than its applications were well recognized by the general community. It is, however, best known as the Wiener index $W(\cdot)$ since its application in chemistry was first proposed in 1947 [32–34]. Along this line other distance-based graph invariants have also been studied. Related references include [2,4–9,14,15,17,19–30,36,38,39]. In particular, distances between leaves, distances between internal vertices, and distances between internal vertices and leaves have also been considered in addition to the Wiener index.

Related to the Wiener index is the *distance function*

$$d_G(v) = \sum_{u \in V(G)} d(u, v),$$

often considered as the "local" version of the Wiener index since

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} d_G(v)$$

for a graph G, where $d(u, v)$ is the distance between the vertices u and v.

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These concepts were extensively studied for trees because of the frequent appearances of acyclic structures (or structures very close to acyclic) in applications. The “middle part” of a tree with respect to such a local function has been studied in [1] long before the related applications were known. In a tree T the set of vertices that minimize the distance function, denoted by $C(T)$ and called the *centroid*, is known to be either a single vertex or two adjacent vertices. For an example of further investigations of middle parts of a tree with respect to various distance functions one may see [31], where centroid, “internal centroid”, and “leaf centroid” of a tree are studied and compared.

The edge version of the Wiener index seems to be first proposed in [18] and studied in [11]. Simply put, the edge-Wiener index W_e of a graph is the sum of distances between all pairs of edges. In recent years many studies have been published on various related problems including extremal questions as well as the relation between the edge version and the original Wiener index [3,10,12,13,16,35,37]. We contribute to this effort by considering the middle parts of a tree with respect to the distance-based functions defined on edges.

We will first introduce several different types of “edge-centroids”, along with their basic properties, in Section 2. Then the characteristics of these different edge-centroids and the structural relations between them are further examined in Section 3. These relations motivated us to consider how far apart different edge-centroids can be from each other. These extremal distances and the corresponding extremal trees are presented in Section 4. Lastly, in Section 5, the centroid and edge-centroid, within the same graph, are studied. Some interesting and perhaps unexpected findings are shown. We comment on our results in Section 6 and propose some directions for potential future studies.

2. Middle parts of a tree defined through edge distances

Recall that the edge-Wiener index of G can be defined as

$$W_e(G) = \sum_{\{f,g\}\subseteq E(G)} d(f,g),$$

where $d(f, g)$ is the distance between the corresponding vertices in the line graph of G. Then the distance function at a vertex is extended to the *edge-distance function* (at an edge)

$$d_e(f) = \sum_{g\in E(G)} d(f,g).$$

As mentioned earlier, the distance (and the corresponding middle parts of a tree) between internal vertices and leaves have also been studied. In the case of distance between edges it is natural to define

$$d_{P_e}(f) = \sum_{g\in P_e(G)} d(f,g)$$

and

$$d_{I_e}(f) = \sum_{g\in I_e(G)} d(f,g)$$

where $P_e(G)$ and $I_e(G)$ denote, respectively, the set of pendant edges and the set of internal edges of G. Analogous to the centroid, internal-centroid, and leaf-centroid that were extensively investigated for trees, we first consider the middle parts *edge-centroid*, *pendant edge-centroid* and *internal edge-centroid*, denoted by $C_E(T)$, $C_{P_e}(T)$ and $C_{I_e}(T)$, defined as the sets of edges of T where $d_e(.)$, $d_{P_e}(.)$ and $d_{I_e}(.)$ are minimized, respectively.

In a more general setting, let F be a function defined on the natural numbers, the “edge-distance function associated with F” is

$$d_F(f) = \sum_{g\in E(G)} F(d(f,g)).$$

It is not hard to see that with different F information on $d_F(\cdot)$ can be useful in further investigations of these edge-distance related problems. We will start with examining the properties of $d_F(\cdot)$ in trees. The structural characteristics of different edge-centroids then follow as corollaries. For an edge $f\in E(G)$, we say that an edge $g\neq f$ is the neighbor of f if g and f have one common vertex in G.

Proposition 2.1. *Let $F(x)$ be nonnegative, strictly increasing and concave up. For any three edges $f_1, f_2, f_3\in E(T)$ such that $f_1 = v_1v_2$, $f_2 = v_2v_3$ and $f_3 = v_3v_4$, we have*

$$2d_F(f_2) < d_F(f_1) + d_F(f_3).$$